COMPLEX HAMILTONIAN DYNAMICS

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Lecture 1:

Introduction to Hamiltonian Dynamics: Stability and Chaos

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Contents

Dynamical Systems and Stability of Equilibrium Points

Dynamical systems in continuous time are described by systems of Ordinary Differential Equations (ODEs), in n real dependent variables $(x_k(t), k = 1, 2, \ldots, n$, which constitute a state $\vec{x}(t) = (x_1(t), \ldots, x_n(t))$ in the phase space of the system $D \subseteq \mathbb{R}^n$ and are functions of the single independent variable of the problem: the time $t \in \mathbb{R}$. Their dynamics is described by the system of first order ODEs

$$\frac{dx_k}{dt} = f_k(x_1, x_2, \ldots, x_n), \quad k = 1, 2, \ldots, n \tag{1}$$

Since the f_k do not explicitly depend on t the system is called autonomous. The functions f_k are defined everywhere in D and are assumed analytic in all their variables, meaning that they can be expressed as convergent series expansions in the x_k (with non-zero radius of convergence) near one of their equilibrium (or fixed) points, located at the origin of phase space $\vec{0} = (0, \ldots, 0) \in D$, where

$$f_k(\vec{0}) = 0, \quad k = 1, 2, \ldots, n. \tag{2}$$

What can we say now about the solutions of these equations in a small neighborhood of the equilibrium point (2), where the series expansions of the f_k converge? Is the motion “regular” or “predictable” there? This is the question of stability of motion first studied systematically by the great Russian mathematician A. M. Lyapunov, more than 110 years ago.

The first and simplest notion of stability is called asymptotic stability and refers to the case where all solutions $x_k(t)$ of (1), starting near the origin, tend to 0 as $t \to \infty$. A less restrictive situation arises when we can prove that for every $0 < \varepsilon < \varepsilon_0$, no matter how small, all solutions starting at $t = t_0$ within a neighborhood of the origin $K(\varepsilon) \subseteqq B(\varepsilon)$, where $B(\varepsilon)$ is a “ball” of radius ε around the origin, remain inside $B(\varepsilon)$ for all $t \geq t_0$.

This so-called neutral or conditional stability will be of great importance to us, as it frequently occurs in conservative dynamical systems, among which are the Hamiltonian systems. These conserve phase space volume and hence cannot come to a complete rest at any value of t, finite or infinite. As we shall discuss later, conditional stability characterizes precisely the systems for which Lyapunov could prove the existence of families of periodic solutions around the origin.

To discuss the question of stability of the motion near an equilibrium point, we need to know something about the behavior of the solutions of the linearized equations about that point. Thus one might try to compare these solutions to an exponential function of time, with the purpose of identifying a particular exponent, which we call today the Lyapunov characteristic exponent (LCE).

Let us identify the meaning of these exponents for our problem. Indeed, they are directly related to the eigenvalues of the $n \times n$ matrix $J = (p_{jk}), j, k = 1, 2, \ldots, n$, obtained as the roots of the characteristic equation

$$\det(J - \lambda I_n) = 0, \tag{3}$$

$\lambda_1, \lambda_2, \ldots, \lambda_n$, I_n being the $n \times n$ identity matrix.

In modern terminology, therefore, consider a dynamical system (1), with an equilibrium point at $(0, 0, \ldots, 0)$ and a constant Jacobian matrix

$$J_{k,j} = p_{kj} = \frac{\partial f_k}{\partial x_j}(0, \ldots, 0)/\ j, k = 1, 2, \ldots, n, \tag{4}$$

The above analysis translates to the following well-known result:

Theorem (see p. 181 Hirsch and Smale, 1974) If all eigenvalues of the matrix J have negative real part less than $-c, \ c > 0$, there is a compact neighborhood U of the origin, such that, for all $(x_1(0), x_2(0), \ldots, x_n(0)) \in U$, all solutions $x_k(t) \to 0$, as $t \to \infty$. Furthermore, one can show that this approach to the fixed point is exponential: Indeed, if we denote by $|\cdot|$ the Euclidean norm in $\mathbb{R}^n$ and define $\vec{x}(t) = (x_1(t), x_2(t), \ldots, x_n(t))$, it can be proved that for all $\vec{x}(0)$ in U, $|\vec{x}(t)| \leq |\vec{x}(0)|e^{-ct}$, and $|\vec{x}(t)|$ is in U for all $t \geq 0$.

Lyapunov paid particular attention to the case where one (or more) of the eigenvalues of the linearized equations have zero real part. This was the beginning of what we now call bifurcation theory, as it constitutes the turning point between stability of the fixed point (all eigenvalues have negative real part) and instability, where at least one eigenvalue has positive real part.

This theory can be found, not only in Lyapunov's treatise "Stability of Motion" but also in a many textbooks on the qualitative theory of ODEs (Hirsch, Smale and Devaney, 2004, Perko, 1995 and Wiggins, 1990). One more result of Lyapunov's theory, concerning simple periodic solutions of Hamiltonian systems, will be described in the next section.

Hamiltonian Systems of N=1 and 2 Degrees of Freedom

Let us now apply the above theory to the case of Hamiltonian dynamical systems of N degrees of freedom (dof), where $n = 2N$ and the equations of motion are

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k}, \quad \frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k}, \quad k = 1, 2, \ldots, N, \tag{5}$$

where $q_k(t)$, $p_k(t)$, $k = 1, 2, \ldots, 2N$ are the position and momentum coordinates and H is the Hamiltonian. If H does not explicitly depend on t, it is a first integral (or constant of the motion), whose value equals the total energy of the system E.
We now assume that our Hamiltonian can be expanded in power series as a sum of homogeneous polynomials H_m of degree $m \geq 2$

$$H = H_2(q_1, \ldots, q_N, p_1, \ldots, p_N) + H_3(q_1, \ldots, q_N, p_1, \ldots, p_N) + \ldots = E, \tag{6}$$

so that the origin is always an equilibrium point of the system. $H(q_k(t), p_k(t)) = E$ thus defines the so-called constant energy surface, on which our Hamiltonian dynamics evolves.

If the linear equations resulting from (5) and (6), with $H_m = 0$ for all $m > 2$, yield a matrix, whose eigenvalues all occur in conjugate imaginary pairs, $\pm i\omega_k$, these provide the frequencies of the normal mode oscillations of the linearized system.

We can then change to normal mode coordinates and write our Hamiltonian in the form of N *uncoupled* harmonic oscillators

$$H^{(2)} = \frac{\omega_1}{2}({x_1}^2 + {y_1}^2) + \frac{\omega_2}{2}(x_2^2 + y_2^2) + \ldots + \frac{\omega_N}{2}(x_N^2 + y_N^2) = E, \tag{7}$$

where $x_k,\ y_k,\ k = 1, 2, \ldots, N$ are the new position and momentum coordinates and ω_k represent the normal mode frequencies of the system.

Theorem (Lyapunov) If none of the ratios of these eigenvalues, ω_j/ω_k, is an integer, for any $j, k = 1, 2, \ldots, N$, $j \neq k$, the linear normal modes continue to exist as periodic solutions of the nonlinear system (5) when higher order terms $H_3, H_4, \ldots$ etc. are taken into account in (6).

These solutions have frequencies close to those of the linear modes and are examples of what we call simple periodic orbits (SPOs), where all variables oscillate with the same frequency $\omega_k = 2\pi/T_k$, returning to the same values after a single maximum (and minimum).

These are also called nonlinear normal modes, or NNMs. As we vary the total energy E in (6) their stability under small perturbations of their initial conditions changes and although a local property, is often relevant for the more global stability properties of the system!

The case of $N = 1$ degree of freedom

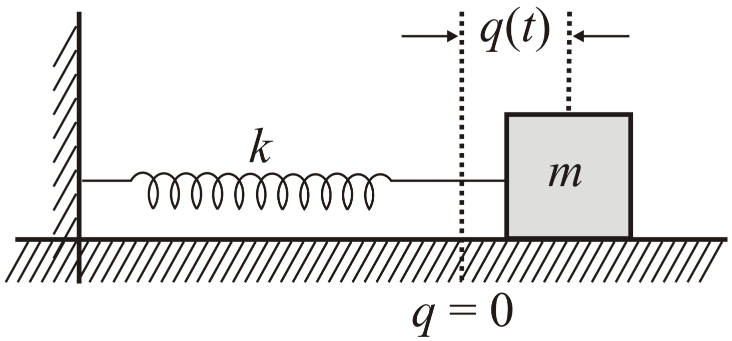
One of the first physical systems that we encounters in our studies is the harmonic oscillator shown in Fig. 9 described by Newton's second order differential equation

$$m\frac{d^2q}{dt^2} = -kq, \tag{8}$$

where $k > 0$ is a constant representing the hardness (or softness) of the spring. Equation (8) can be easily solved to yield the displacement $q(t)$ as an oscillatory function of time of the form

$$q(t) = A\sin(\omega t + \alpha), \quad \omega = \sqrt{k/m}, \tag{9}$$

where A and α are free constants corresponding to the amplitude and phase of oscillations and ω is the frequency.



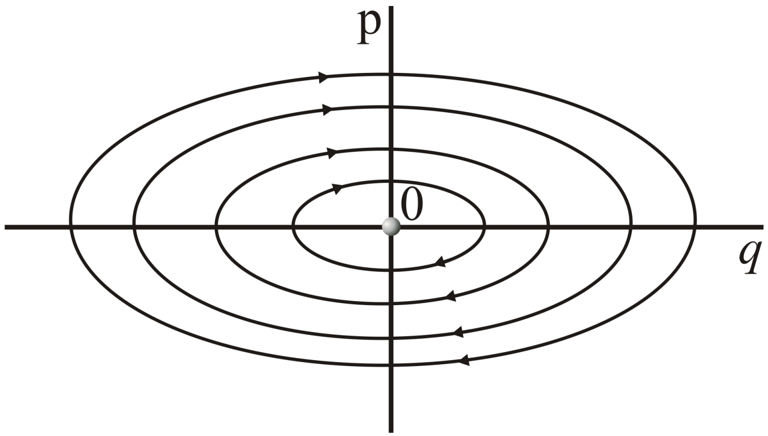
If we now recall that $p = m dq/dt$ represents the momentum of the mass m, we rewrite (8) in the form of two first order ODEs

$$\frac{dq}{dt} = \frac{p}{m} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -kq = -\frac{\partial H}{\partial q}, \tag{10}$$

derived from the $N = 1$ dof Hamiltonian function

$$H(q, p) = \frac{p^2}{2m} + k\frac{q^2}{2} = E, \tag{11}$$

which represents the total (kinetic plus potential) energy. If we plot the solutions as orbits in the (q, p) phase space we obtain the curves shown below, where $q(t)$ and $p(t)$ oscillate periodically with the same frequency ω.



A nonlinear system of N=1 degrees of freedom

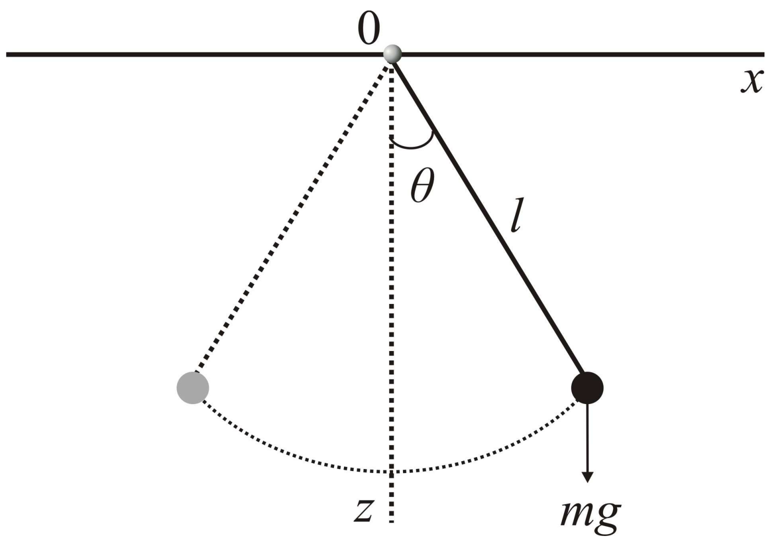
A more interesting one dof Hamiltonian system representing the motion of a simple pendulum shown in Fig. 11. Its equation of motion is

$$ml^2 \frac{d^2\theta}{dt^2} = -mlg \sin\theta, \tag{12}$$

If we now write this equation as a system of two first order ODEs, we find again that they can be cast in Hamiltonian form

$$\frac{dq}{dt} = p = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{g}{l} \sin q = -\frac{\partial H}{\partial q}, \tag{13}$$

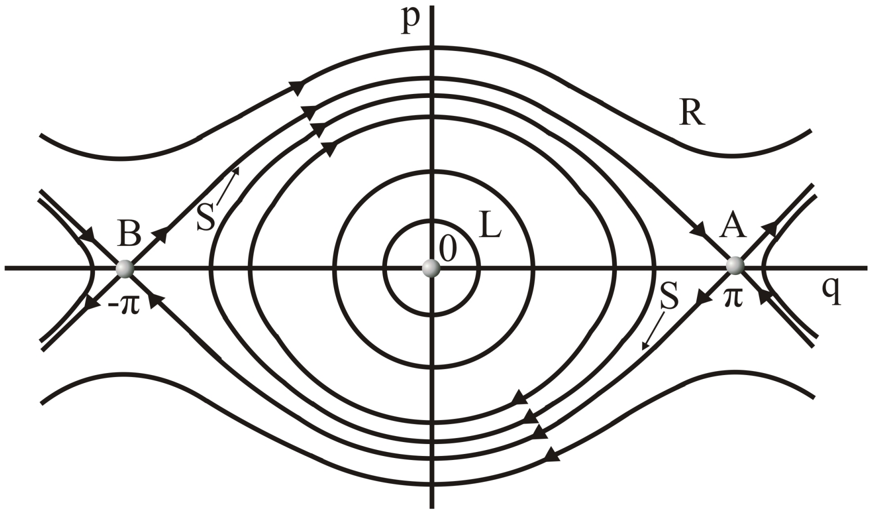
where $q = \theta$.



In this case, the energy integral is

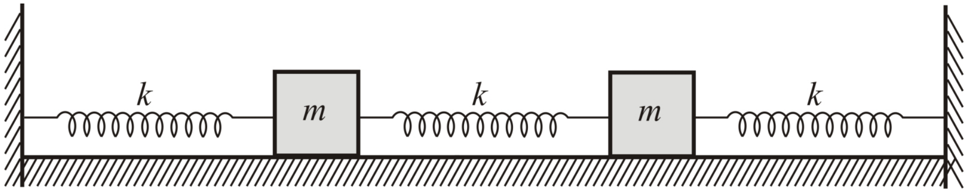
$$H(q,p) = \frac{p^2}{2} + \frac{g}{l}(1 - \cos q) = E. \tag{14}$$

Plotting this family of curves in the (q,p) phase space for different values of E we now obtain a much more interesting picture than Fig. 10 depicted in Fig. 12 below. Observe that, besides the elliptic fixed point at the origin, there are two new equilibria located at the points $(\pm\pi, 0)$. These points A and B are called saddle points and are unstable in contrast to the $(0,0)$ fixed point, which is stable characterized by what we called conditional (or neutral) stability.



The case of N=2 degrees of freedom: Integrability and chaos

Let us extend our study to Hamiltonian systems of two dof, joining at first two harmonic oscillators, as shown in Fig. 13. We shall assume that our oscillators have equal masses $m_1 = m_2 = m$ and spring constants $k_1 = k_2 = k$ and impose fixed boundary conditions to their endpoints.



Newton's equations of motion give in this case:

$$m\frac{d^2q_1}{dt^2} = -kq_1 - k(q_1 - q_2), \quad m\frac{d^2q_2}{dt^2} = -kq_2 + k(q_1 - q_2), \tag{15}$$

where $q_i(t)$ are the particles' displacements from their equilibrium positions at $q_i = 0$, $i = 1, 2$. If we also introduce the momenta $p_i(t)$ of the two particles in terms of their velocities, we obtain the Hamiltonian function

$$H(q_1, p_1, q_2, p_2) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + k\frac{q_1^2}{2} + k\frac{q_2^2}{2} + k\frac{(q_1 - q_2)^2}{2} = E \tag{16}$$

If we now change variables

$$Q_1 = \frac{q_1 + q_2}{\sqrt{2}}, \quad Q_2 = \frac{q_1 - q_2}{\sqrt{2}}, \quad P_1 = \frac{p_1 + p_2}{\sqrt{2}}, \quad P_2 = \frac{p_1 - p_2}{\sqrt{2}} \tag{17}$$

we see that, adding and subtracting by sides the two equations in (15) (dividing also by m and introducing $\omega = \sqrt{k/m}$), splits the problem into two uncoupled harmonic oscillators

$$\frac{dQ_i}{dt} = \frac{P_i}{m}, \quad \frac{dP_i}{dt} = -\omega_i^2 Q_i, \quad i = 1, 2, \quad \omega_1 = \omega, \quad \omega_2 = \sqrt{3}\omega, \tag{18}$$

with frequencies ω_1, ω_2. The new Hamiltonian of the system

$$K(Q_1, P_1, Q_2, P_2) = \frac{P_1^2}{2m} + \frac{P_2^2}{2m} + k\frac{Q_1^2}{2} + 3k\frac{Q_2^2}{2} = E. \tag{19}$$

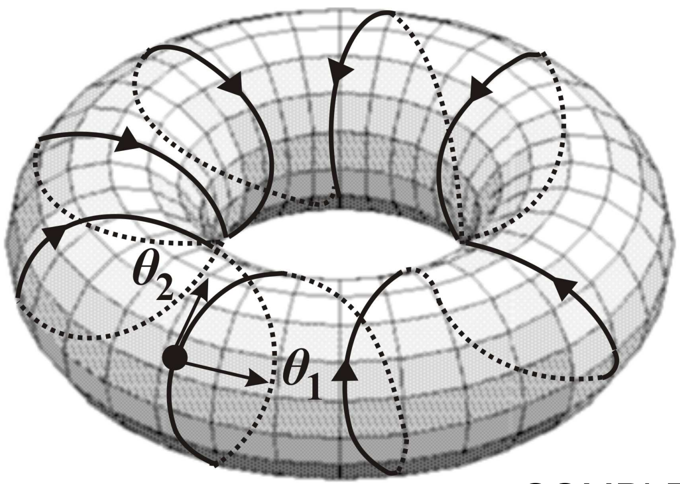
is expressed as the sum of the Hamiltonians of these oscillators. Thus, changing variables we have performed a canonical coordinate transformation and realize that our system possesses two integrals of the motion

$$F_i(Q_1, P_1, Q_2, P_2)) = \frac{P_i^2}{2m} + k_i\frac{Q_i^2}{2} = E_i, \quad i = 1, 2, \tag{20}$$

with $k_1 = k$, $k_2 = 3k$, while E_i are two free parameters of the system to be fixed by the initial conditions $q_i(0)$, $p_i(0)$, $i = 1, 2$.

The solutions of this system are, in general, linear combinations of trigonometric functions with frequencies $\omega_1 = \sqrt{k}$, $\omega_2 = \sqrt{3k}$. If these were rationally dependent, i.e. if their ratio were a rational number $\omega_1/\omega_2 = m_1/m_2$ $(m_1, m_2$ all orbits close on 2-dimensional invariant tori and the motion would be periodic. In our example, this could only happen for initial conditions such that E_1 or E_2 is zero.

For E_1 and E_2 both non-zero the oscillations are quasiperiodic, as they are the superposition of trigonometric terms whose frequencies are rationally independent, since the ratio $\omega_2/\omega_1 = \sqrt{3}$ is irrational. Hence, the orbits in the 4-dimensional phase space are never closed, i.e. they never pass by the same point and eventually cover uniformly a 2-dimensional torus specified by the values of E_1 and E_2.



A nonlinear system of N=2 degrees of freedom

We now turn to a system of two coupled nonlinear oscillators connected with the famous Hénon and Heiles Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(\omega_1^2 q_1^2 + \omega_2^2 q_2^2) + q_1^2 q_2 - \frac{C}{3} q_2^3. \tag{21}$$

describing the motion of a star of mass m in the axisymmetric potential of a galaxy. Introducing the more convenient variables $q_1 = x$, $q_2 = y$, $p_1 = p_x$, $p_2 = p_y$, we rewrite the above Hamiltonian in the form

$$H = \frac{1}{2}(p_x^2 + p_y^2) + V(x, y) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(Ax^2 + By^2) + x^2 y - \frac{C}{3} y^3 = E, \tag{22}$$

where E is the total energy and we have set $\omega_1^2 = A > 0$ and $\omega_2^2 = B > 0$. Newton's equations of motion associated with this system are

$$\frac{d^2 x}{dt^2} = -\frac{\partial V}{\partial x} = -Ax - 2xy, \quad \frac{d^2 y}{dt^2} = -\frac{\partial V}{\partial y} = -By - x^2 + Cy^2. \tag{23}$$

Note that (22) represents a first integral of this system. If we could also find a second one, the problem would be completely integrable and could be integrated by quadratures. This, however, is highly unlikely in general!

The surprising result is there are only 3 known cases in which a second integral exists, allowing one to solve the Hénon-Heiles equations completely:

$$\begin{aligned} \text{Case } 1: &\quad A = B, \quad C = -1, \\ \text{Case } 2: &\quad A, B \text{ free}, \quad C = -6, \\ \text{Case } 3: &\quad B = 16A, \quad C = -16. \end{aligned} \tag{24}$$

In these cases, most orbits (in phase space domains of bounded motion) would be quasiperiodic and lie on 2-dimensional tori rendering the dynamics perfectly regular and predictable. For all other parameter values, one finds (besides periodic and quasiperiodic orbits), a new kind of solution that appears "irregular" and "unpredictable", which we call chaotic. These solutions tend to occupy densely 3-dimensional regions in the 4-dimensional phase space and depend very sensitively on initial conditions, in the sense that almost all other orbits in their vicinity deviate exponentially from the chaotic orbit as time increases.

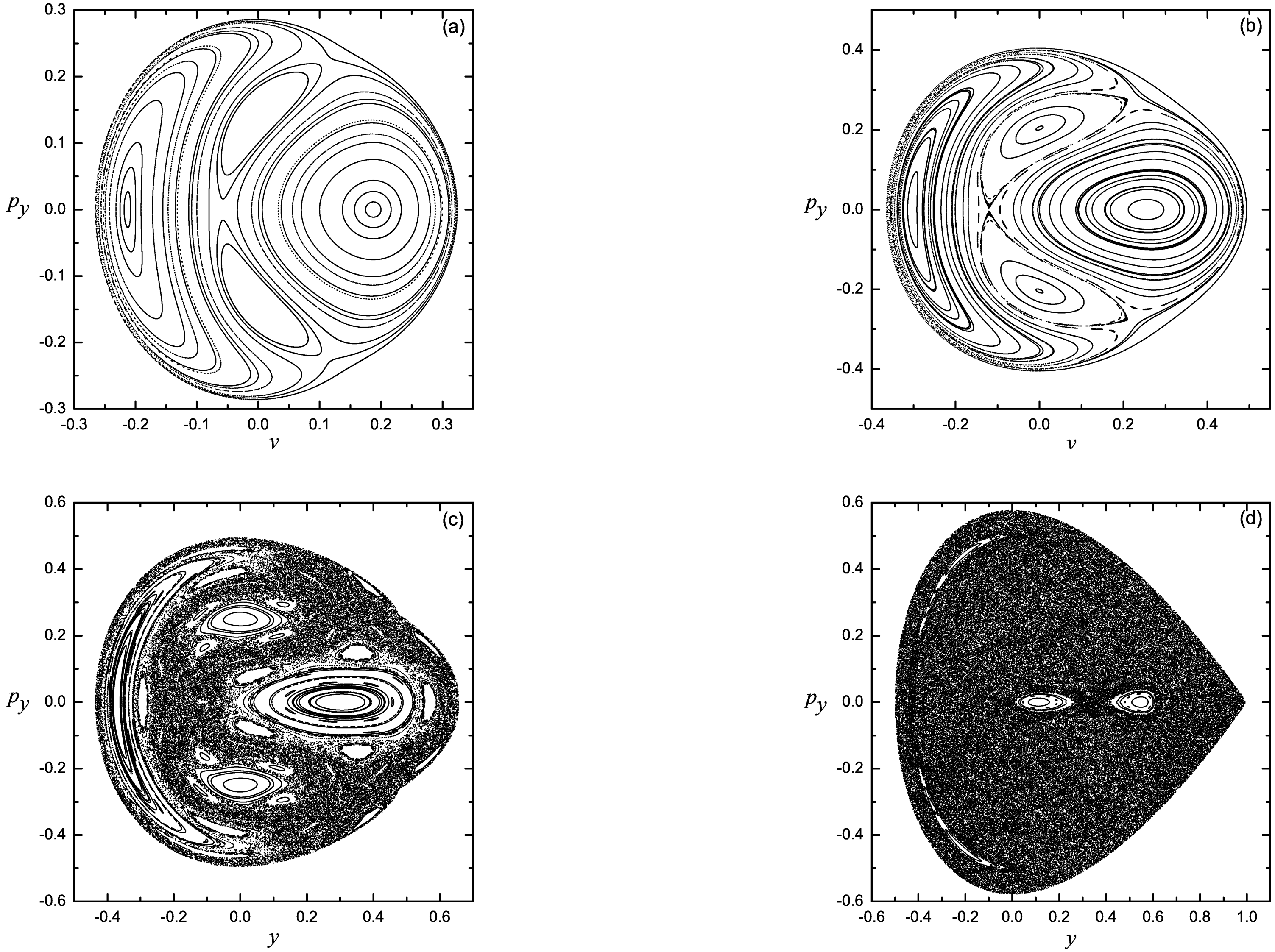


Figure 1: On the Poincare Surface of Section (y, p_y) for (a) $E = 1/24$ and (b) $E = 1/12$, no chaotic orbits are visible. At (c) $E = 1/8$, we observe islands of order surrounded by chaos. In (d), where $E = 1/6$, chaotic motion extends over most of phase space.

Stability Analysis of Periodic Orbits

To discuss the stability of periodic orbits, we need two fundamental concepts: The first is more analytical and is provided by Floquet theory and the second is more numerical and refers to the so-called Poincaré map and its associated surfaces of section (PSS).
In particular, we will assume that our n-dimensional dynamical system, cast in the general form $\dot{\vec{x}} = \vec{f}(\vec{x})$ (see (1)) has a periodic solution $\hat{\vec{x}}(t) = \hat{\vec{x}}(t+T)$ of period T. Let us choose an arbitrary point along this orbit $\hat{\vec{x}}(t_0)$ and define a PSS at that point as follows

$$\Sigma_{t_0} = \left\{ \vec{x}(t) \ \ / \ \ (\vec{x}(t) - \hat{\vec{x}}(t_0)) \cdot \vec{f}(\hat{\vec{x}}(t_0)) = 0 \right\}. \tag{25}$$

Thus, Σ_{t_0} is a $(n-1)$-dimensional plane which intersects the given periodic orbit at $\hat{\vec{x}}(t_0)$ and is vertical to the direction of the flow at that point. Clearly now a Poincaré map can be defined on that plane as before, by

$$P : \Sigma_{t_0} \to \Sigma_{t_0}, \quad \vec{x}_{k+1} = P\vec{x}_k, \quad k = 0, 1, 2, \ldots \tag{26}$$

for which $\vec{x}_0 = \hat{\vec{x}}(t_0)$ is a fixed point, since $\vec{x}_0 = P\vec{x}_0$.

We now examine small deviations about this point,

$$\vec{x}_k = \hat{\vec{x}}_0 + \vec{\eta}_k, \quad ||\vec{\eta}_k|| \ll \varepsilon, \tag{27}$$

(where ε is of the same magnitude as $||\hat{\vec{x}}_0||$), substitute (27) in (26) and linearize the Poincaré map to obtain

$$\vec{\eta}_{k+1} = DP(\hat{\vec{x}}_0)\vec{\eta}_k, \tag{28}$$

where we have neglected higher order terms in $\vec{\eta}$ and $DP(\hat{\vec{x}}_0)$ denotes the Jacobian of P evaluated at $\hat{\vec{x}}_0$.
To determine P we may use the *variational equations* of the original differential equations derived by writing $\vec{x}(t) = \hat{\vec{x}}(t) + \vec{\xi}(t)$, whence linearizing (1) about this periodic orbit leads to the system

$$\dot{\vec{\xi}}(t) = A(t)\vec{\xi}(t), \quad A(t) = A(t+T), \tag{29}$$

where $A(t)$ is the Jacobian matrix of $\vec{f}(\vec{x})$ evaluated at the periodic orbit $\vec{x}(t) = \hat{\vec{x}}$. The crucial question, of course, we must face now is: How are the two linear systems (28) and (29) related to each other?

Observe that we have used different notations for the small deviations about the periodic orbit: $\vec{\xi}(t)$ in the continuous time setting of differential equations and $\vec{\eta}_k$ in the discrete time setting of the Poincaré map. This is to emphasize that their dimensionality as vectors in the n-dimensional phase space $\mathbb{R}^n$ ($n = 2N$ for a Hamiltonian system) is different: $\vec{\xi}(t)$ is n-dimensional, while $\vec{\eta}_k$ is $(n-1)$-dimensional! How are we to match these two small deviation variables?

The answer will come from what is called Floquet theory (see Perko, 1995,Wiggins, 1990). First we realize that since (29) is a linear system of ODEs it must possess, in general, n linearly independent solutions, forming the columns of the $n \times n$ *fundamental solution* matrix $M(t, t_0)$ in

$$\vec{\xi}(t) = M(t, t_0)\vec{\xi}(0), \quad M(t, t_0) = M(t + T, t_0) \tag{30}$$

Now, if we change our basis at the point $\hat{\vec{x}}(t_0)$ so that one of the directions of motion is along the direction *vertical* to the PSS (25), we will observe that the nth column of the matrix $M(T, t_0)$ has zero elements except at the last entry which is 1. Thus, if we eliminate from this matrix its nth row and nth column, it turns out that its $(n-1) \times (n-1)$ submatrix is none other than our beloved Poincaré map (26)!

This means that if we could compute the so-called monodromy matrix $M(T, t_0)$ numerically we could evaluate its eigenvalues, $\mu_1, \ldots, \mu_{n-1}$ (the last one being $\mu_n = 1$), which are those of the Poincaré map and determine the stability of our periodic orbit as follows: If they are all on the unit circle, i.e. $|\mu_i| = 1, \;\; i = 1, \ldots, n-1$, the periodic orbit is (linearly) stable, while if (at least) one of them satisfies $|\mu_j| > 1$ the periodic solution is unstable.

But how do we compute the monodromy matrix $M(T, t_0)$? It is not so difficult. Let us first set $t_0 = 0$ for convenience and observe from (30) that $M(0, 0) = I_n$. All we have to do is integrate numerically the variational equations (30) from $t = 0$ to $t = T$, n times, each time for a *different* initial vector $(0, \ldots, 0, 1, 0, \ldots, 0)$ with 1 placed in the ith position, $i = 1, 2, \ldots, n$.

Note that since these equations are linear numerical integration can be performed to *arbitrary accuracy* and is also not too-time consuming for reasonable values of the period T. Once we have calculated $M(T, 0)$, we may proceed to compute its eigenvalues and determine the stability of the periodic orbit according to whether at least one of these eigenvalues has magnitude greater than 1.

The Fermi–Pasta–Ulam (FPU)-β model

The FPU -β one-dimensional lattice is described by the Hamiltonian

$$H = \frac{1}{2}\sum_{j=1}^{N}\dot{x}_j^2 + \sum_{j=0}^{N}\left(\frac{1}{2}(x_{j+1}-x_j)^2 + \frac{1}{4}\beta(x_{j+1}-x_j)^4\right) = E \tag{31}$$

Let us focus on **Simple Periodic Orbits**(SPOs), where all variables oscillate in or out of phase and return to their initial state after only one maximum and one minimum in their oscillation. The SPOs we consider here are:

I. The FPU π-mode under periodic boundary conditions:

$$x_{N+k}(t) = x_k(t),\ \forall t, k \tag{32}$$

where the particles execute out-of-phase motion (OPM) with N even

$$\hat{x}_j(t) = -\hat{x}_{j+1}(t) \equiv \hat{x}(t),\ j = 1, \ldots, N. \tag{33}$$

II. For the FPU model and fixed boundary conditions:

$$x_0(t) = x_{N+1}(t) = 0, \ \forall t \tag{34}$$

(a) **The SPO1 mode**, with N odd,

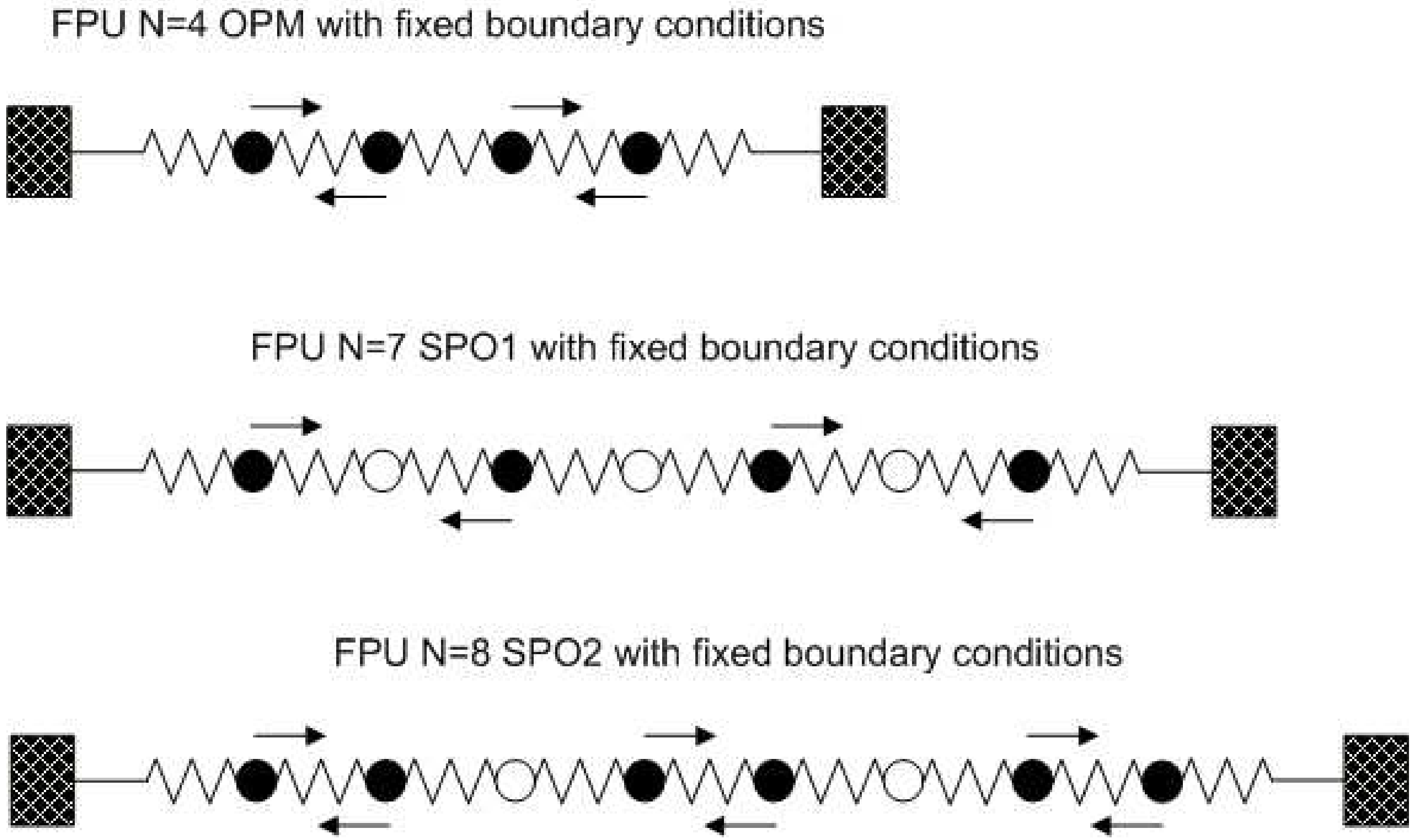
$$\hat{x}_{2j}(t) = 0, \ \hat{x}_{2j-1}(t) = -\hat{x}_{2j+1}(t) \equiv \hat{x}(t), \ j = 1, \ldots, \frac{N-1}{2}. \tag{35}$$

(b) **The SPO2 mode**, with $N = 5 + 3m, \ m = 0, 1, 2, \ldots$ particles,

$$x_{3j}(t) = 0, \ j = 1, 2, 3 \ldots, \frac{N-2}{3}, \tag{36}$$

$$x_j(t) = -x_{j+1}(t) = \hat{x}(t), \ j = 1, 4, 7, \ldots, N-1. \tag{37}$$

Let us see some of these solutions graphically in the figure of the next page:


FPU N=4 OPM with fixed boundary conditions
FPU N=7 SPO1 with fixed boundary conditions
FPU N=8 SPO2 with fixed boundary conditions

An application of Floquet stability analysis

Stability analysis of SPOs is performed by studying the eigenvalues of the monodromy matrix. To see how this is done consider the SPO1 mode of FPU, for which the equations of motion collapse to a single second order ODE:

$$\ddot{\hat{x}}(t) = -2\hat{x}(t) - 2\beta\hat{x}^3(t) \tag{38}$$

Its solution is well–known in terms of Jacobi elliptic functions

$$\hat{x}(t) = \mathcal{C}\,\mathrm{cn}(\lambda t, \kappa^2) \tag{39}$$

with modulus κ^2. Linearizing about this solution $x_j = \hat{x}_j + y_j$, by keeping up to linear terms in y_j, we get the variational equations

$$\ddot{y}_j = (1 + 3\beta\hat{x}^2)(y_{j-1} - 2y_j + y_{j+1}),\ j = 1, \ldots, N \tag{40}$$

These separate into N uncoupled Lamé equations

$$\ddot{z}_j(t) + 4(1 + 3\beta\hat{x}^2)\sin^2\left(\frac{\pi j}{2(N+1)}\right) z_j(t) = 0,\ j = 1, \ldots, N \tag{41}$$

where the z_j variations are simple linear combinations of the y_j's.

Changing variables to $u = \lambda t$, the above equation takes the form

$$z_j''(u) + 2\big(1 + 4\kappa^2 - 6\kappa^2 \mathrm{sn}^2(u,\kappa^2)\big)\sin^2\left(\frac{\pi j}{2(N+1)}\right) z_j(u) = 0,\ j = 1,\ldots,N \tag{42}$$

where primes denote differentiation with respect to u. According to Floquet theory, its solution is bounded (or unbounded) depending on whether the eigenvalues of the monodromy matrix are **on or off the unit circle**.

These periodic solutions all experience a first destabilization at energy densities:

$$\frac{E_c}{N} \propto N^{-\alpha},\ \alpha = 1,\ or,\ 2,\ N \to \infty. \tag{43}$$

More specifically, the first variation $z_j(u)$ to become unbounded as κ^2 (or, the energy E) increases is $j = \frac{N-1}{2}$ and the energy values $E_c/N \propto 1/N$ at which this happens are plotted below.

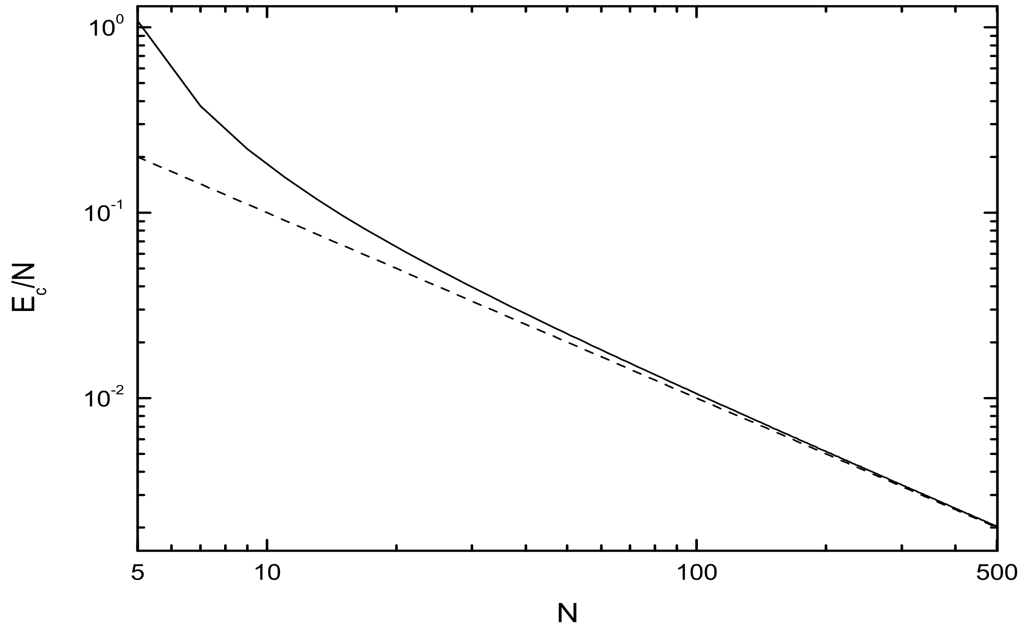


Figure 2: $\frac{E_c}{N}$ of the first destabilization of the SPO1 solution of the FPU system (**the** $k = (N+1)/2$ **mode**) obtained by the monodromy eigenvalues. The dashed line is the function $\propto \frac{1}{N}$.

The OPMs of the FPU and BEC Hamiltonians become unstable, as the eigenvalues of their monodromy matrix exit the unit circle on the real axis: For FPU at -1 (period–doubling bifurcation) and for BEC at +1 (pitchfork bifurcation). Remarkably enough, the IPM of the BEC Hamiltonian **does not destabilize**, no matter what N or E we tried.

An Analytical Criterion for "Weak" Chaos

It was shown very recently by Flach et al. (2005) that the linear modes of the FPU β – model can be continued as SPOs of the corresponding lattice. In fact, the energy threshold for the destabilization of the **low k - modes** ($k = 1, 2, 3, ..$) coincides with the "weak" chaos threshold shown by de Luca and Lichtenberg (1995) to be associated with the **breakup of the famous FPU recurrences**. By k–modes, we refer here to the linear normal modes of the FPU lattice

$$Q_k = \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} q_i \sin \frac{ki\pi}{N+1}, \qquad P_k = \dot{Q}_k \tag{44}$$

with energies and frequencies

$$E_k = \frac{1}{2}\left[P_k^2 + {\omega_k}^2 Q_k^2\right], \;\; \omega_k = 2\sin\frac{k\pi}{2(N+1)} \tag{45}$$

Using linear stability analysis, Flach et al. (2005) report an approximate formula for the destabilization energy of the **low** $k = 1, 2, 3, ..$ **modes** given by

$$E_c \approx \frac{\pi^2}{6\beta(N+1)}. \tag{46}$$

We have discovered that this energy threshold also **coincides** with the instability threshold of our SPO2 mode! In Figure 3 we compare formula (22) (dashed line) with the destabilization threshold for our SPO2 and find excellent agreement.

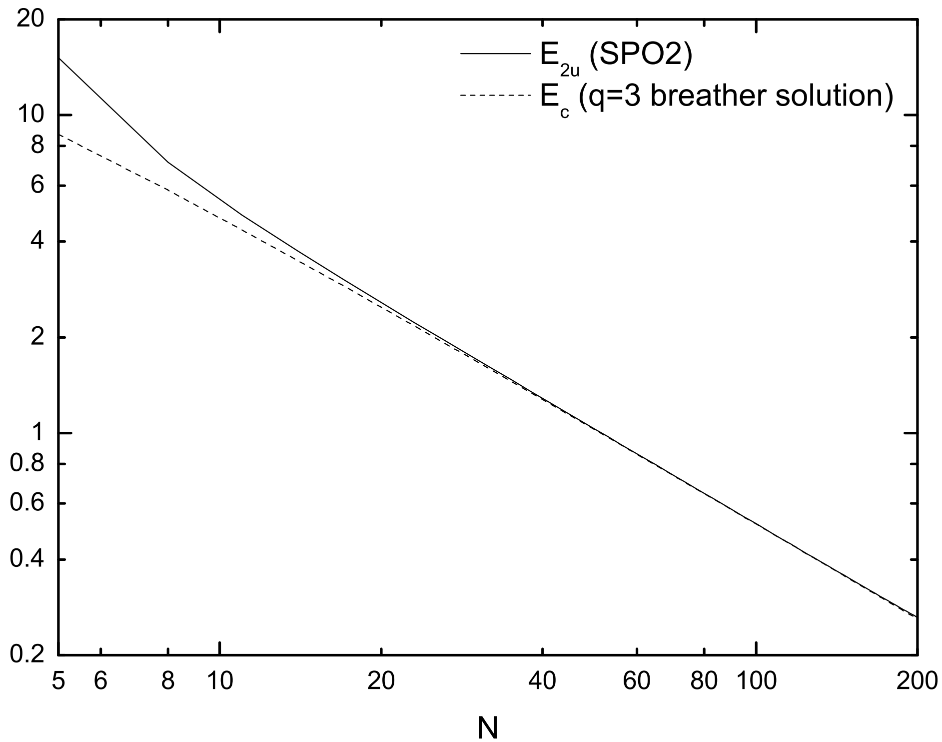


Figure 3: The solid curve is the energy E_c/N of the first destabilization of the SPO2 (**the** $k = 2(N+1)/3$ **mode**) for $\beta = 0.0315$ obtained from the eigenvalues of the monodromy matrix and the dashed line is the approximate formula.

Spectrum of Lyapunov Exponents and “Strong” Chaos

Convergence of Lyapunov Spectra

We now evaluate, in the neighborhood of our SPOs the **Lyapunov spectra**:

$$L_i,\ i = 1, \ldots, 2N,\ L_1 \equiv L_{\max} > L_2 > \ldots > L_{2N}. \tag{47}$$

If the largest one, $L_1 \equiv L_{\max} > 0$, the orbit is chaotic. In particular, we compute in the limit $t \to \infty$ the quantities

$$K_t^i = \frac{1}{t}\ \ln \frac{\| \ \vec{w}_i(t)\ \|}{\| \ \vec{w}_i(0)\ \|}, \tag{48}$$

where $\vec{w}_i(0)$ and $\vec{w}_i(t),\ i = 1, \ldots, 2N$ are deviation vectors from the given orbit $\vec{x}(t)$. After every T_j, following the Bennetin et al.(1980) algorithm, we ortho–normalize the vectors $\vec{w}_i(t)$ and obtain finally L_i by

$$L_i = \lim_{t \to \infty} \frac{1}{n} \sum_{j=1}^{n} K_{T_j}^i,\ n \to \infty. \tag{49}$$

Observe that in the figure below we have plotted the Lyapunov spectrum of **both the OPM and the SPO1 mode** of the FPU Hamiltonian for $N = 16$ and **periodic boundary conditions** at the energy $E = 6.82$ where both of them are unstable. We see that the two Lyapunov spectra are very close to each other suggesting that the chaotic regions are “connected".

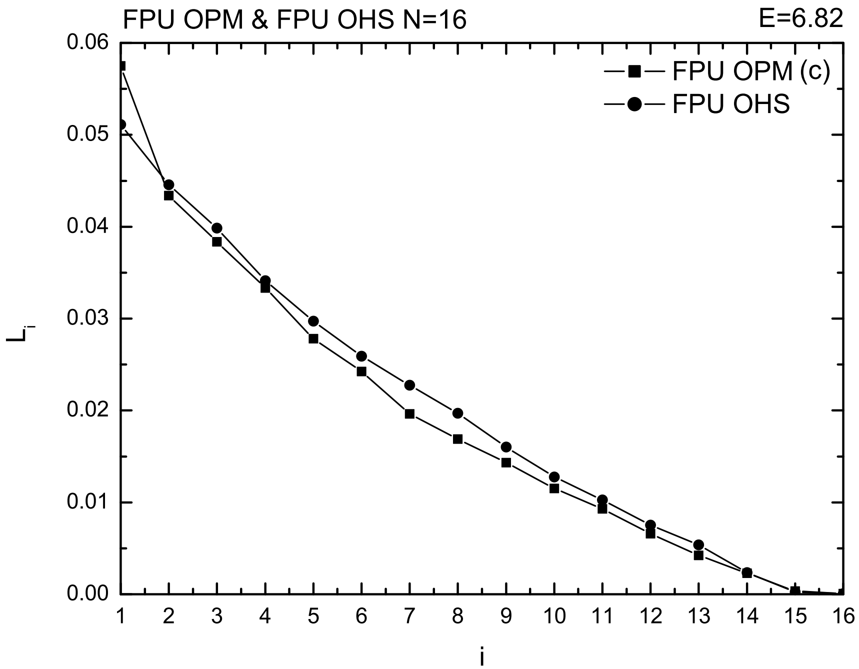
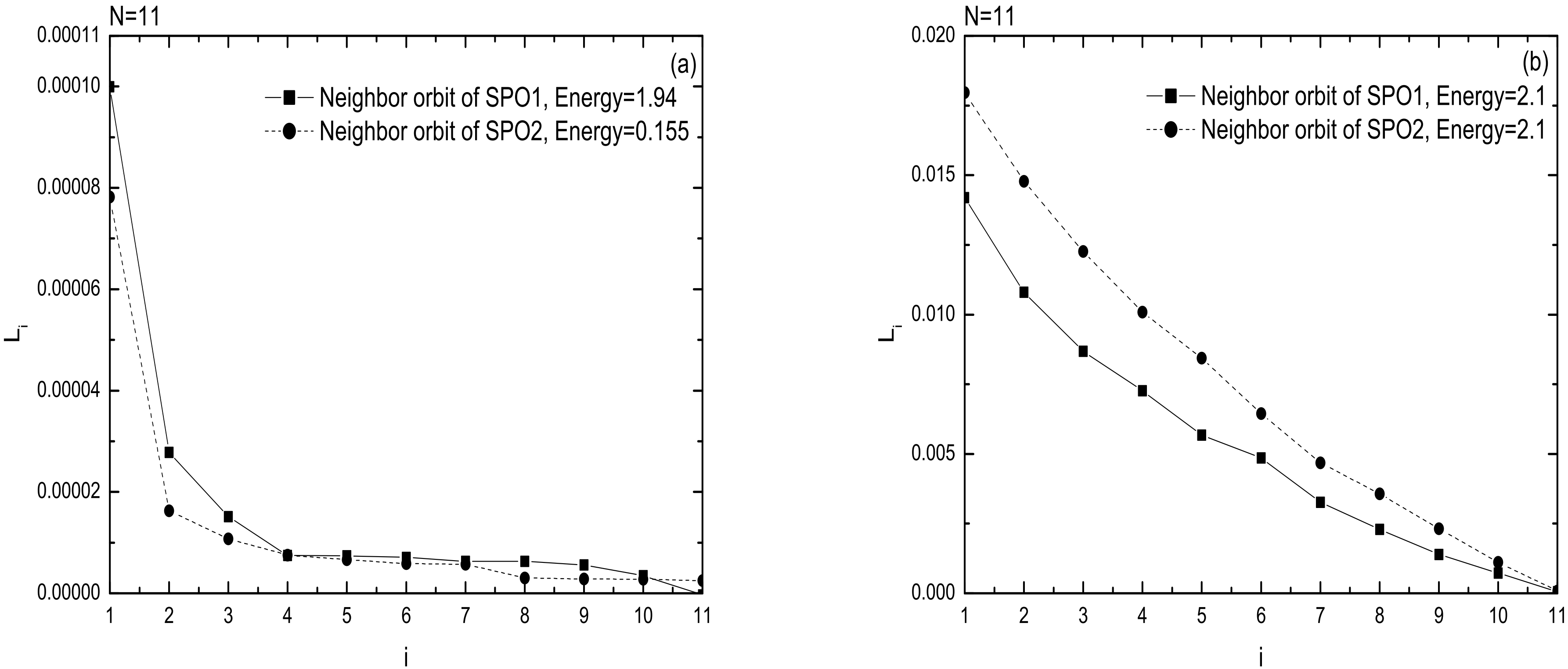


Figure 5: Lyapunov spectra of the OPM and the SPO1 modes of FPU, for $N = 16$ and periodic boundary conditions practically coincide at $E = 6.82$ where both are unstable.

More systematically, let us plot the Lyapunov spectra near the SPO1 and SPO2 modes, of the FPU system, for $N = 11$, **fixed boundary conditions** and energy values $E_1 = 1.94$ and $E_2 = 0.155$ respectively, where the SPOs have just destabilized.



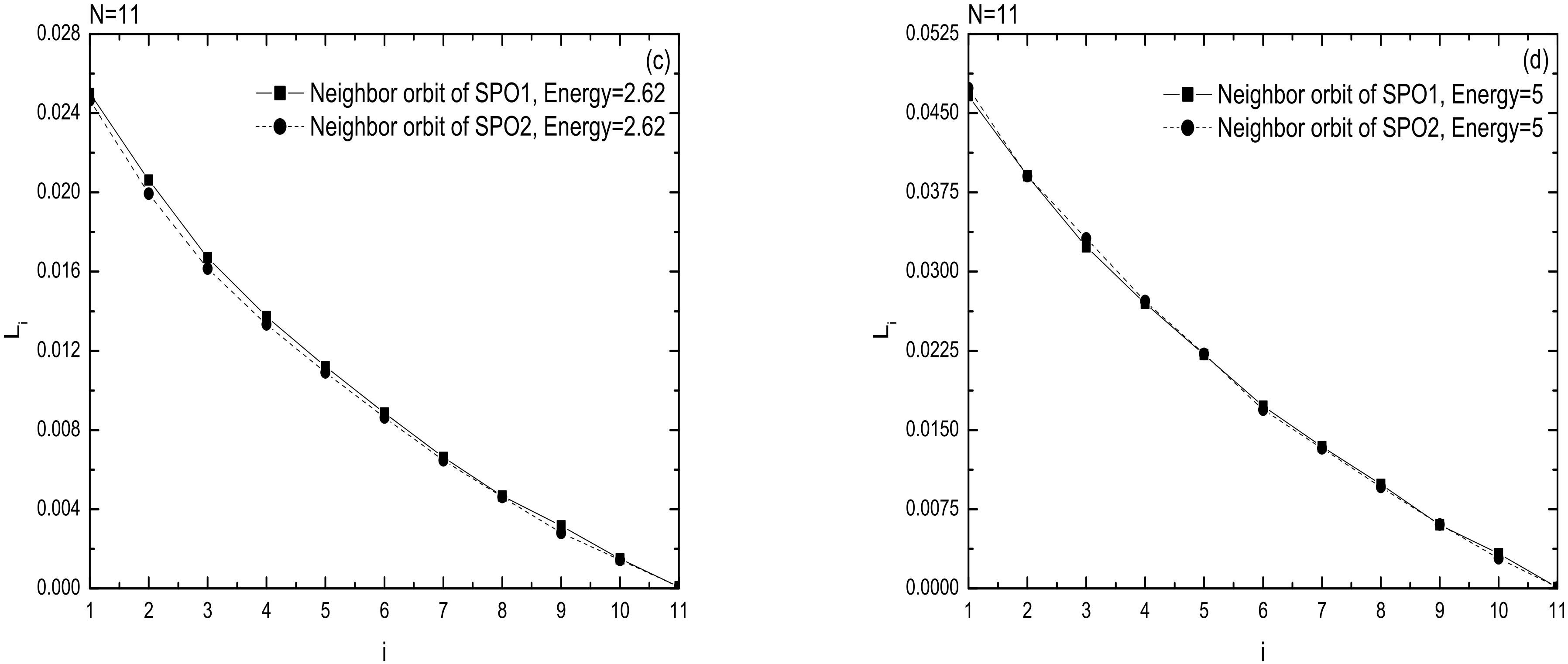


Figure 6: Lyapunov spectra near SPO1 and SPO2 for $N = 11$ at energies $E = 1.94$ and $E = 0.155$, where they have just destabilized. (b) Same as (a) at energy $E = 2.1$. (c) Convergence of the Lyapunov spectra near the two SPOs at energy $E = 2.62$. (d) Coincidence of Lyapunov spectra continues at higher energy $E = 4$.

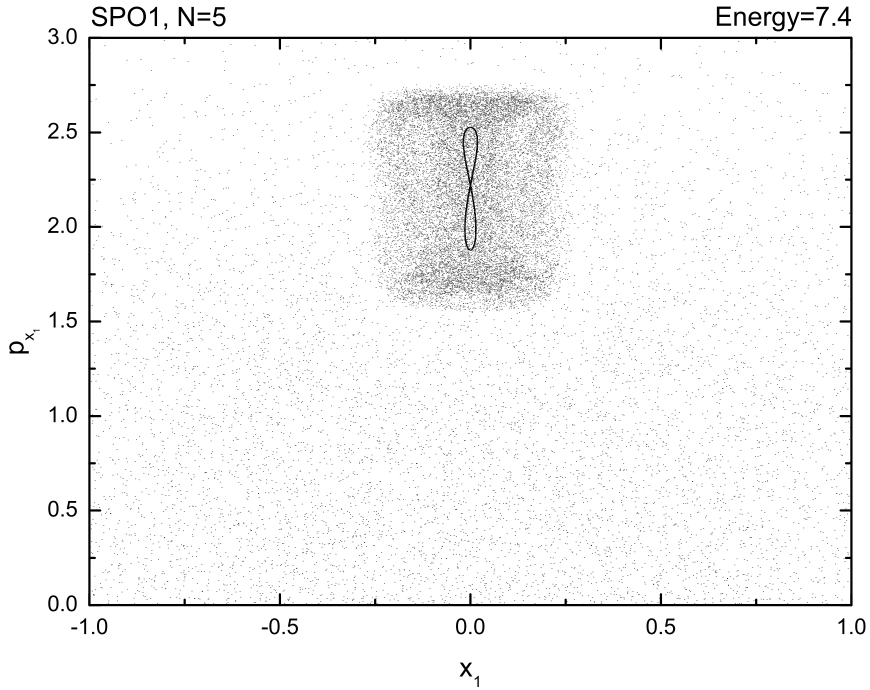


Figure 7: The “figure eight” chaotic region for initial conditions in the immediate vicinity of SPO1 ($\simeq 10^{-5}$), a vague resemblance to “figure eight” for initial conditions a little further away ($\simeq 10^{-1}$) and a large scale chaotic region in the energy surface for initial conditions more distant ($\simeq 1$) for $N = 5$ particles, when it is unstable, on the Poincaré surface of section $(x_1, \dot{x}_1)$ taken at times when $x_3 = 0$. In this picture we integrated our orbits up to $t_n = 10^5$ in the energy surface $E = 7.4$.

Lyapunov Spectra and K-S Entropy

Thus, raising the energy, we observe that at $E = 2.62$, the two spectra have nearly converged to the same exponentially decreasing function,

$$L_i(N) \propto e^{-\alpha \frac{i}{N}}, i = 1, 2, \ldots, K(N) \tag{50}$$

at least up to $K(N) \approx \frac{3N}{4}$. The α exponents for the SPO1 and SPO2 are found to be approximately 2.3 and 2.32 respectively. The figure also shows that this coincidence of Lyapunov spectra persists at higher energies.

Lyapunov Spectra and the Thermodynamic Limit

We can now determine statistical properties of the dynamics in the so–called thermodynamic limit of E and N growing indefinitely, for E/N constant. First, we compute the Lyapunov spectra of the FPU and BEC systems near unstable OPM solutions, which are well approximated by $L_i \propto e^{-\alpha i/N}$.

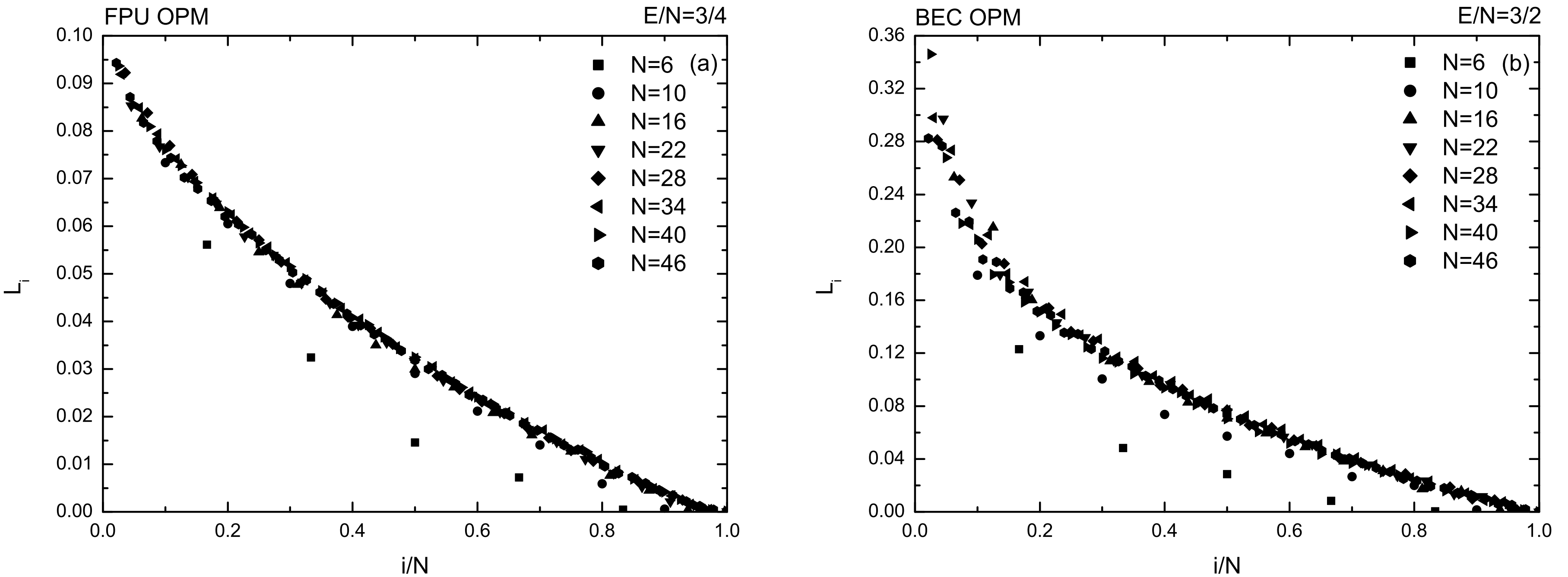


Figure 8: Positive Lyapunov exponents spectrum of the OPM of the FPU Hamiltonian for $E/N = 3/4$. (b) Positive Lyapunov exponents spectrum of the OPM of the BEC Hamiltonian for $E/N = 3/2$.

Specifically, we compute the Kolmogorov–Sinai entropy $h_{KS}(N)$ (solid curves), defined by,

$$h_{KS}(N) = \sum_{i=1}^{N-1} L_i(N), \; L_i(N) > 0. \tag{51}$$

Thus, we find, for both Hamiltonians, that $h_{KS}(N)$ is an **extensive thermodynamic quantity** as it is clearly seen to grow linearly with N, i.e.,

$$h_{KS}(N) = L_{max} \frac{\exp^{-\alpha/N}}{1-\exp^{-\alpha/N}} \approx L_{max} \frac{N}{\alpha} \propto N \tag{52}$$

hence the FPU and BEC Hamiltonians behave as ergodic systems of statistical mechanics.

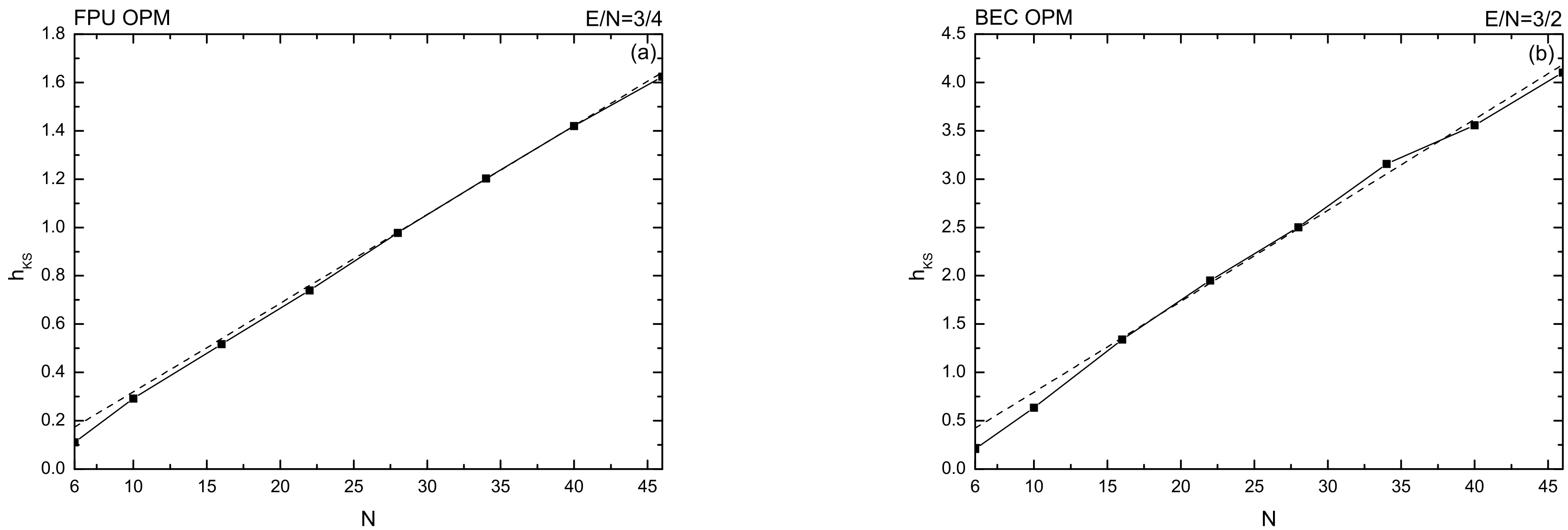


Figure 9: (a) The $h_{KS}(N)$ entropy of the FPU Hamiltonian for fixed $E/N = 3/4$. (b) and of the BEC Hamiltonian for $E/N = 3/2$ (solid curve).

Conclusions

1) We studied local and global dynamics of N dof Hamiltonian systems, focusing on simple periodic orbits (SPOs) and showed that their first destabilization typically decays as

$$E_c/N \propto N^{-\alpha},\ \alpha = 1,\ or,\ 2. \tag{53}$$

2) We showed in the FPU $\beta-$ model that a relatively high $k = 2(N+1)/3$ mode of the linear lattice, is as important for the global dynamics as the low modes, since its destabilization threshold,

$$E_c \approx \frac{\pi^2}{6\beta(N+1)}. \tag{54}$$

coincides with the one found by other researchers for the breakdown of FPU recurrences ("weak" chaos).

3) We calculated the Lyapunov spectra in the vicinity of our SPOs solutions and observed that, as E increases, they attain same functional form,

$$L_i(N) \propto e^{-\alpha \frac{i}{N}}, i = 1, 2, \ldots, K(N) \tag{55}$$

and eventually converge, implying that the corresponding chaotic regions have "merged" and large scale chaos has spread in the system.

4) We thus showed that the associated Kolmogorov–Sinai entropies per particle increase linearly with N

$$h_{KS}(N) = \sum_{i=1}^{N-1} L_i(N) \propto N, \;\; L_i(N) > 0. \tag{56}$$

in the thermodynamic limit of $E \to \infty$ and $N \to \infty$ and fixed E/N and, therefore, behave as extensive quantities of statistical mechanics.

References

1. Skokos, Ch. [2001], “Alignment Indices: A New, Simple Method for Determining the Ordered or Chaotic Nature of Orbits", *J. Phys. A*, **34**, pp. 10029 – 10043.

2. Skokos, Ch., Antonopoulos, Ch., Bountis, T. C. and Vrahatis, M. N. [2003], “How does the Smaller Alignment Index (SALI) Distinguish Order from Chaos?", *Prog. Theor. Phys. Supp.*, **150**, pp. 439 – 443

3. Skokos, Ch., Antonopoulos, Ch., Bountis, T. C. and Vrahatis, M. N. [2004], “Detecting Order and Chaos in Hamiltonian Systems by the SALI Method", *J. Phys. A*, **37**, pp. 6269 – 6284.

4. Antonopoulos, Ch., Bountis, T. C. and Skokos, Ch., [2006], “Chaotic Dynamics of N–Degree–of–Freedom Hamiltonian Systems”, International Journal of Bifurcation and Chaos, vol.**16**(6), 1777-1793 , June 2006.

5. Antonopoulos, Ch. and Bountis, T., [2006], “Stability of Simple Periodic Orbits and Chaos in an FPU Lattice”, PRE**73**, 056206, 1-8 (2006).

6. T. Bountis, "Stability of Motion: From Lyapunov to N - Degree of Freedom Hamiltonian Systems", [2006], "Nonlinear Phenomena and Complex Systems", vol. **9**(3) ,209 -239, 2006.

7. Skokos, Ch., Bountis, T. and Antonopoulos, Ch. [2007], “Geometrical properties of local dynamics in Hamiltonian systems: the Generalized Alignment Index (GALI) method”, Physica D **231**, 30.